Tools for Predicting Exposure Potential

Thomas E. McKone

Lawrence Berkeley National Laboratory

and

University of California, Berkeley

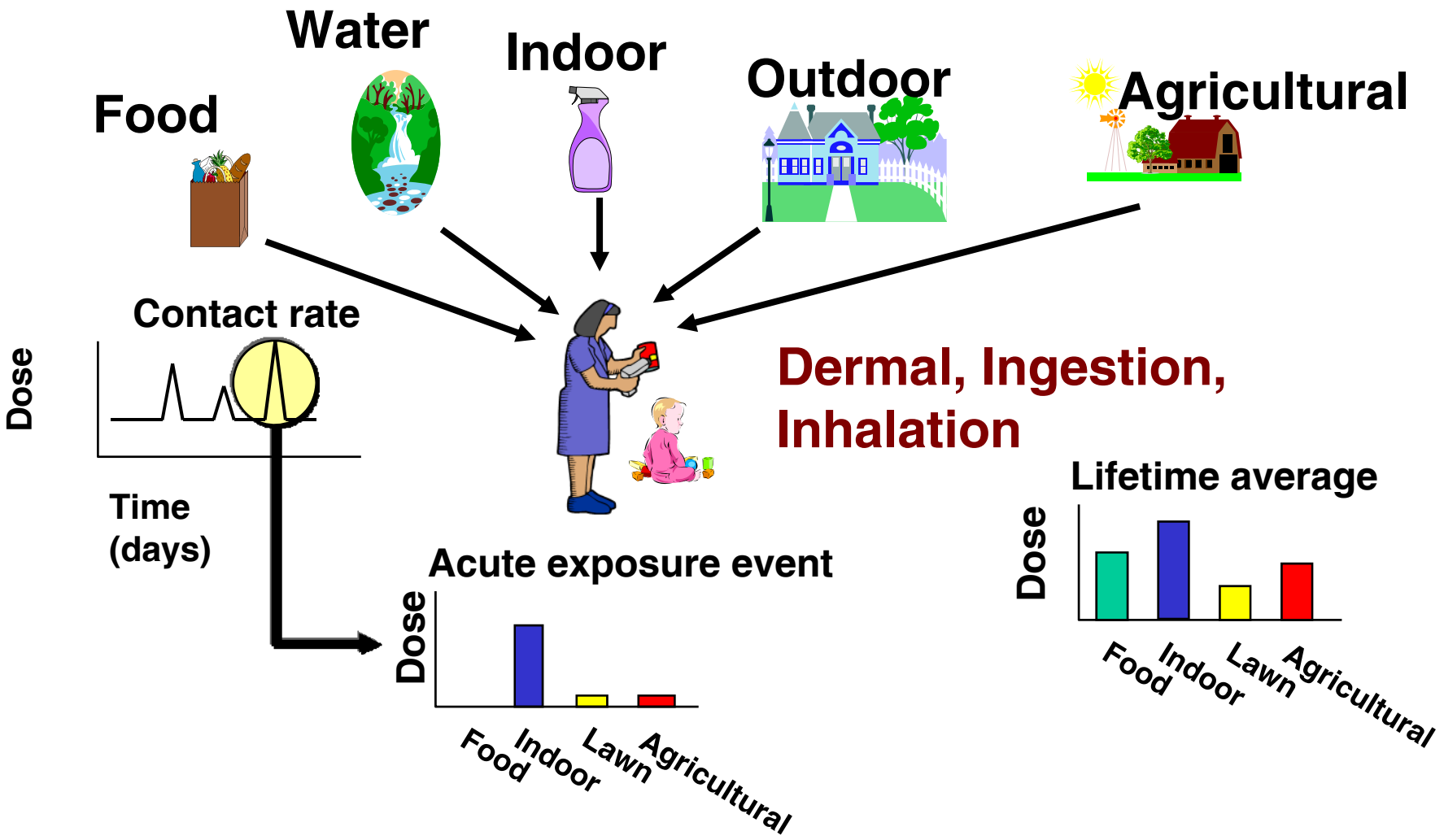
Overview

- Elements of Exposure Assessment
- Persistence, Proximity, and Mobility
- Chemical Properties and Exposure Potential
- Ranking Tools

Exposure Assessment

- **Cumulative Exposures**
  - **Multiple sources**
  - **Multiple pathways**
  - **Multiple routes (inhalation ingestion, dermal)**
- **Dimensions and metrics**
- **Biomonitoring**
- **Models needed to fill information gaps**

Chemical intake depends on release location, transport and fate, and human intake through competing exposure pathways

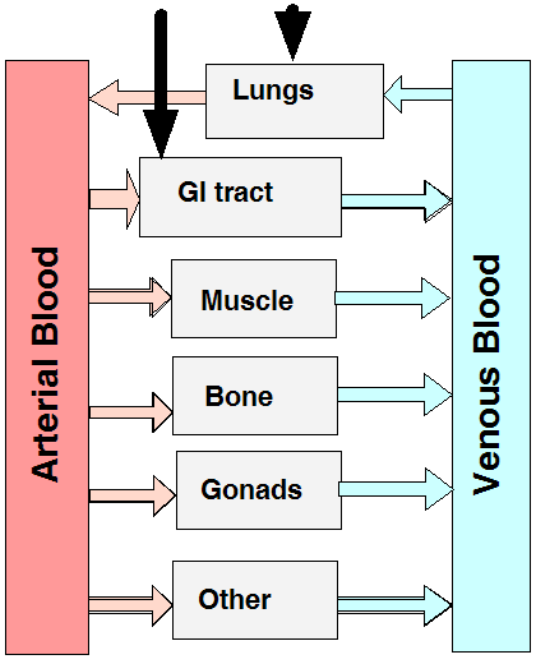


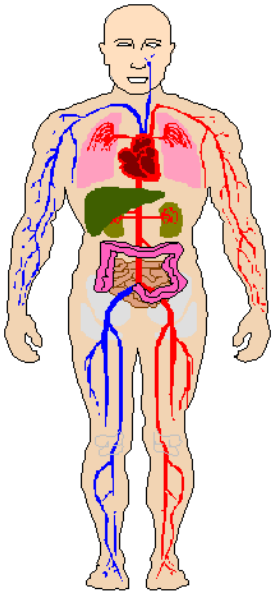
Measures of Exposure

- Population/pollutant classification
- Time-weighted average concentration
- Peak exposure
- Cumulative intake or dose
  - Hour
  - Day
  - Year
- Intake/source ratios
  (Intake fraction)

Biomarkers/Biomonitoring

- **Biomarkers**
  - **Susceptibility**
  - **Exposure**
  - **Effect**
- **Biological media**
  - **Breath**
  - **Saliva**
  - **Urine**
  - **Blood**
  - **Other--lipid samples, biopsies**

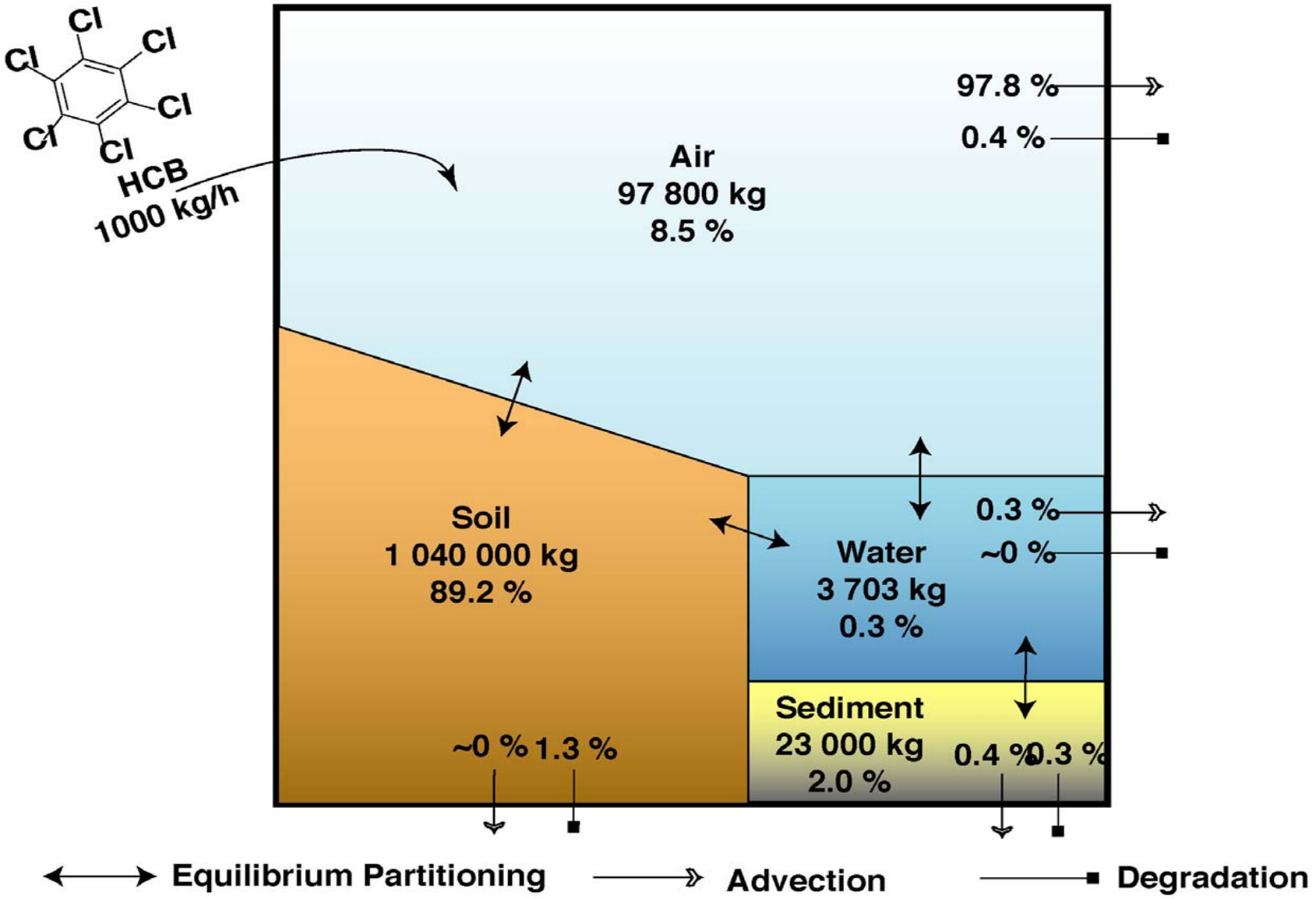




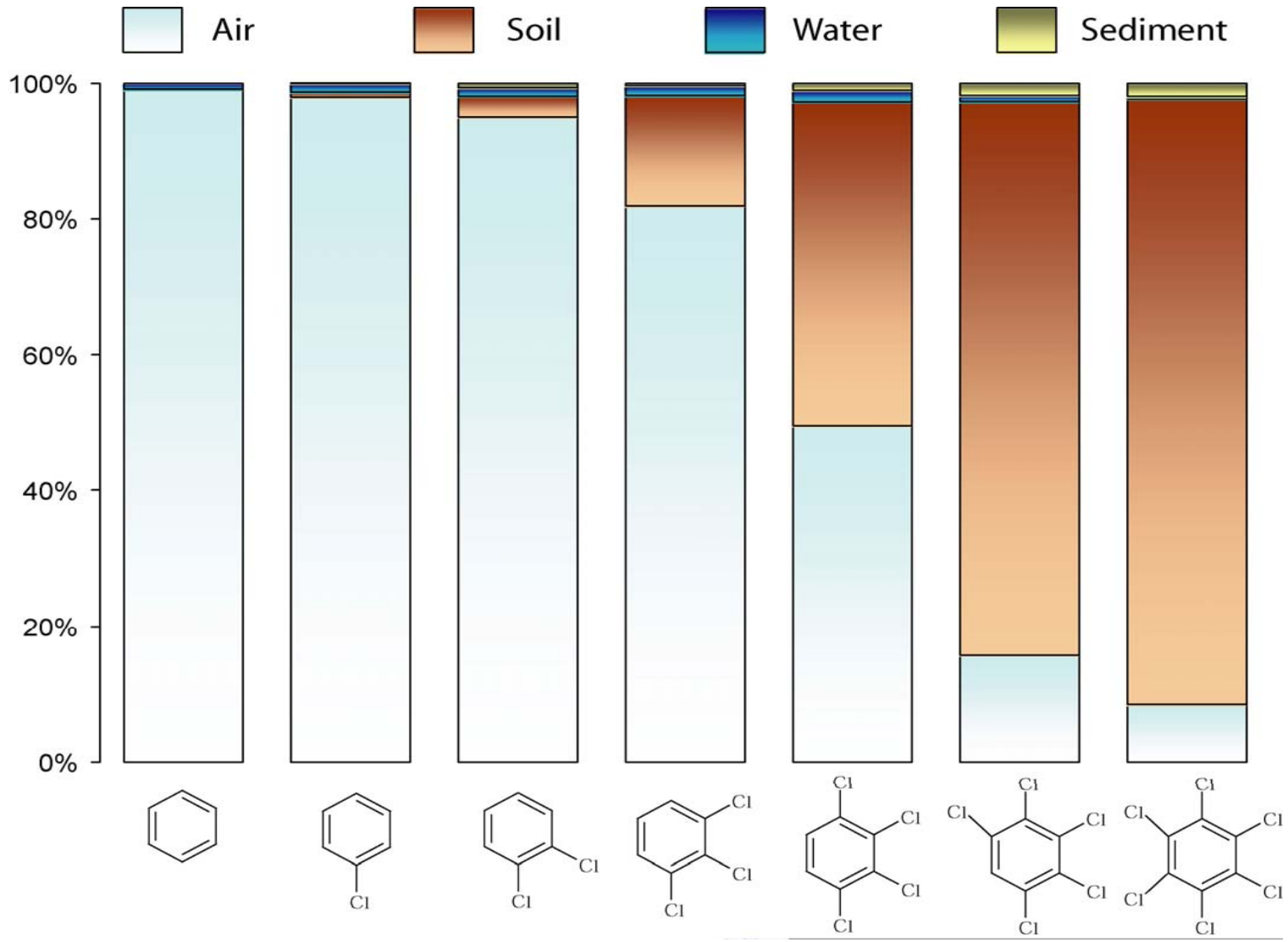
Models Fill Information Gaps

- **Multimedia Mass-Balance Models**
- **Multi-pathway exposure models**
- **Example showing the integration of models and biomarkers**

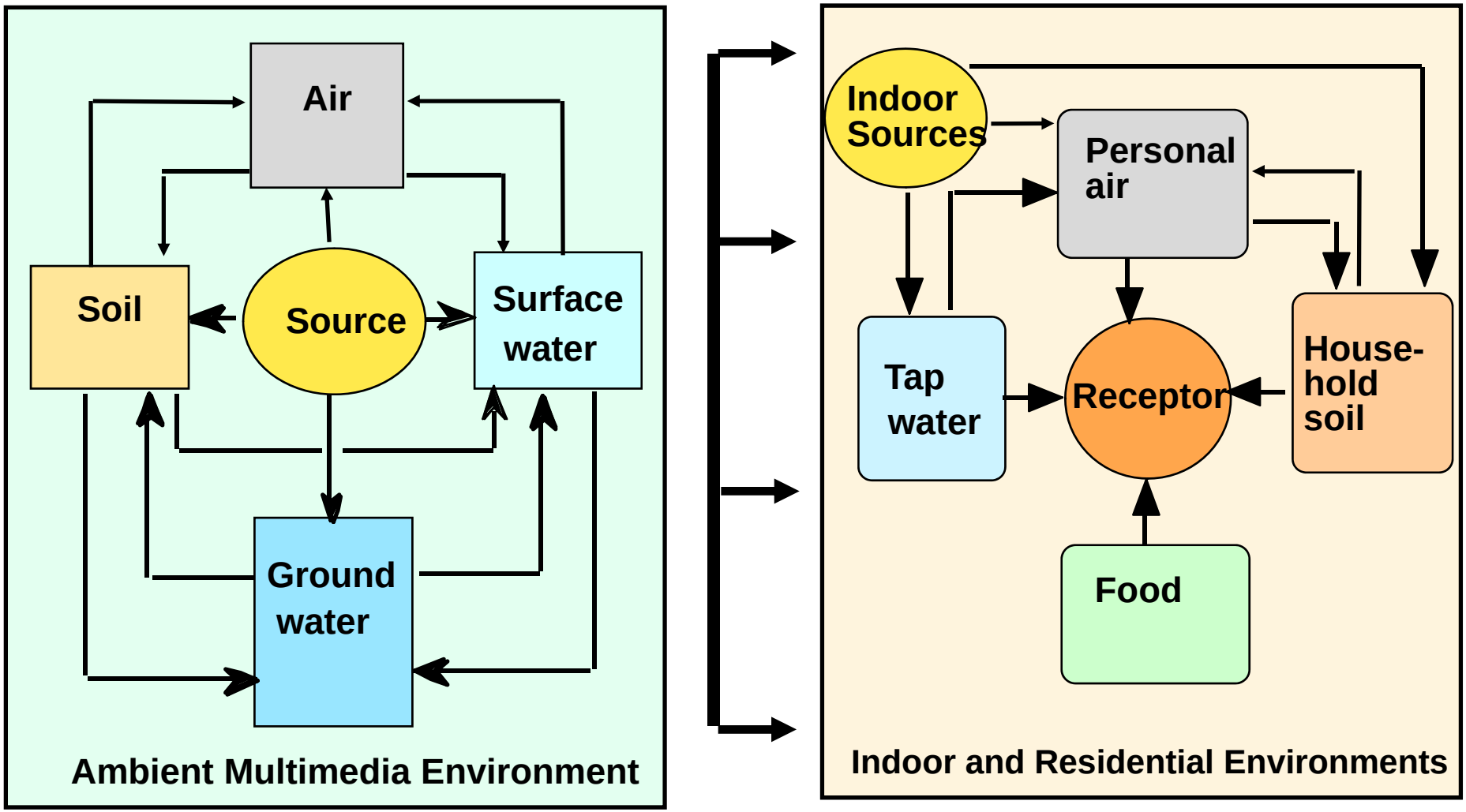
Multimedia Mass Balance Models



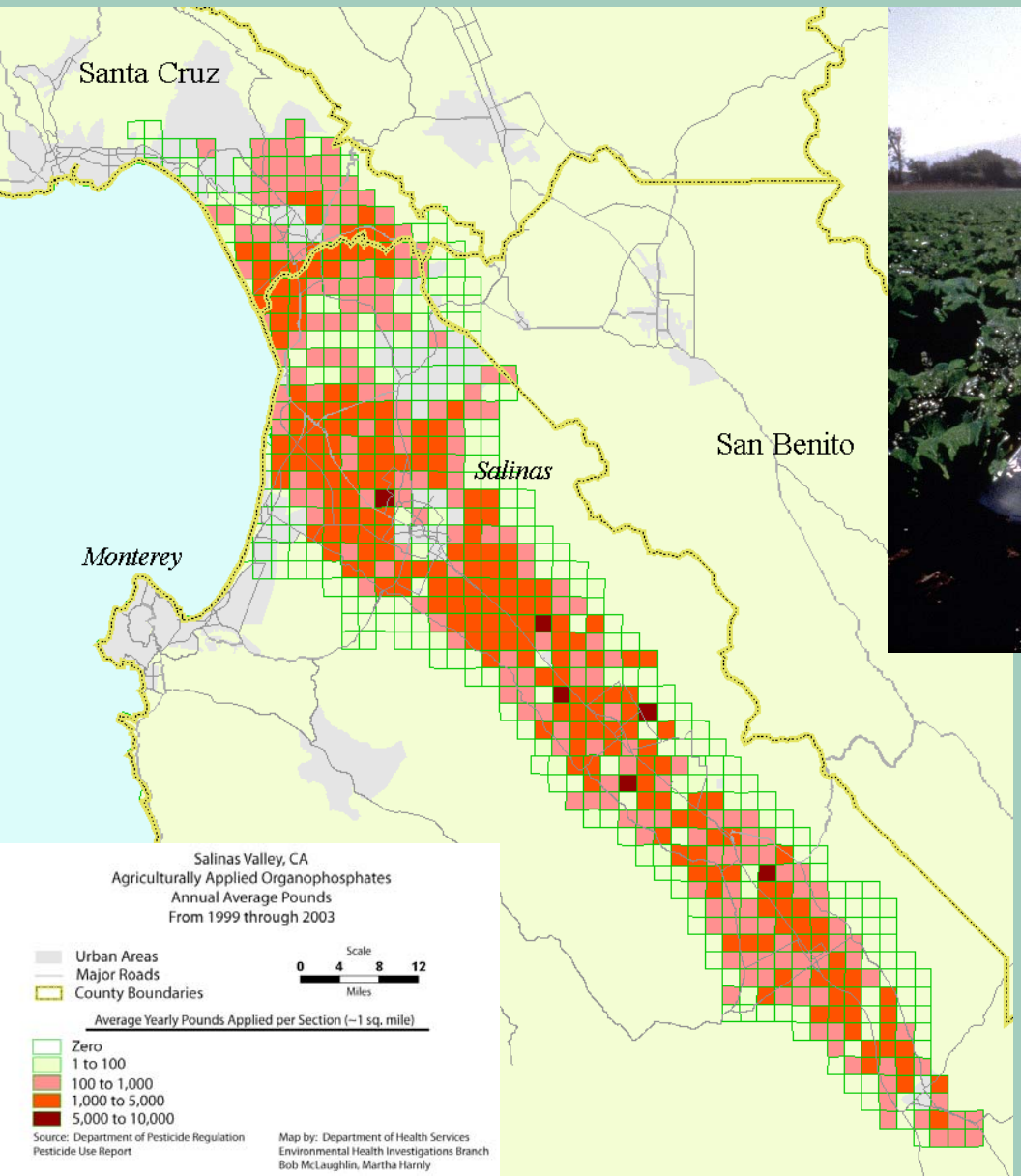
Chlorinated Benzene Series



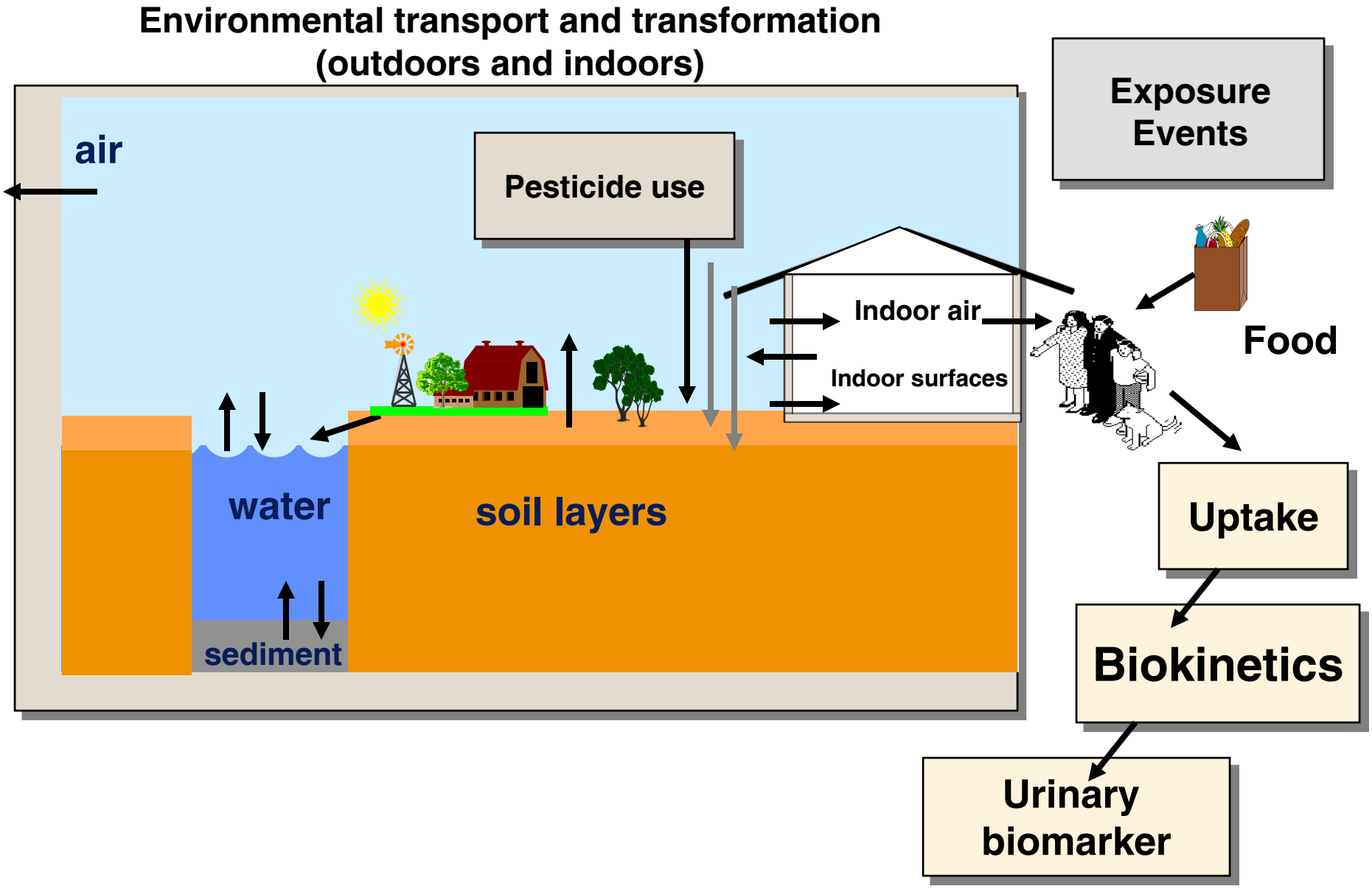
Environmental Media/Exposure Media



Organophosphate Pesticide Use

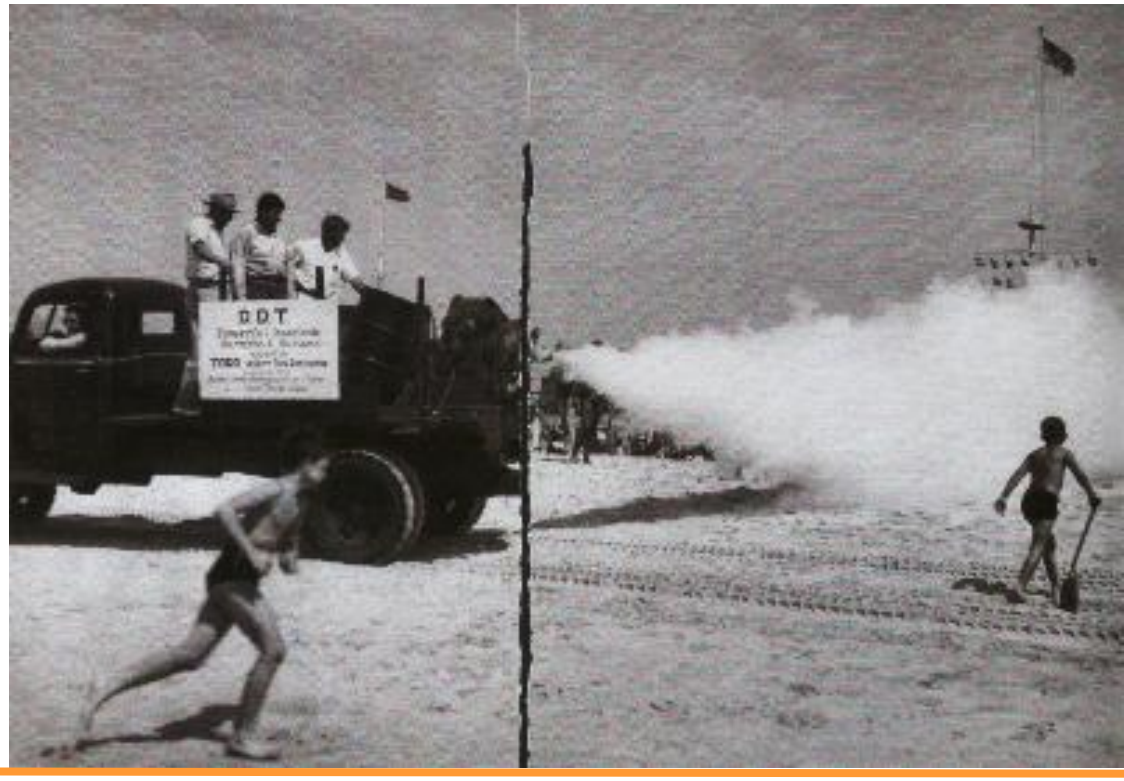


The Salinas Valley is a region of intense pesticide use

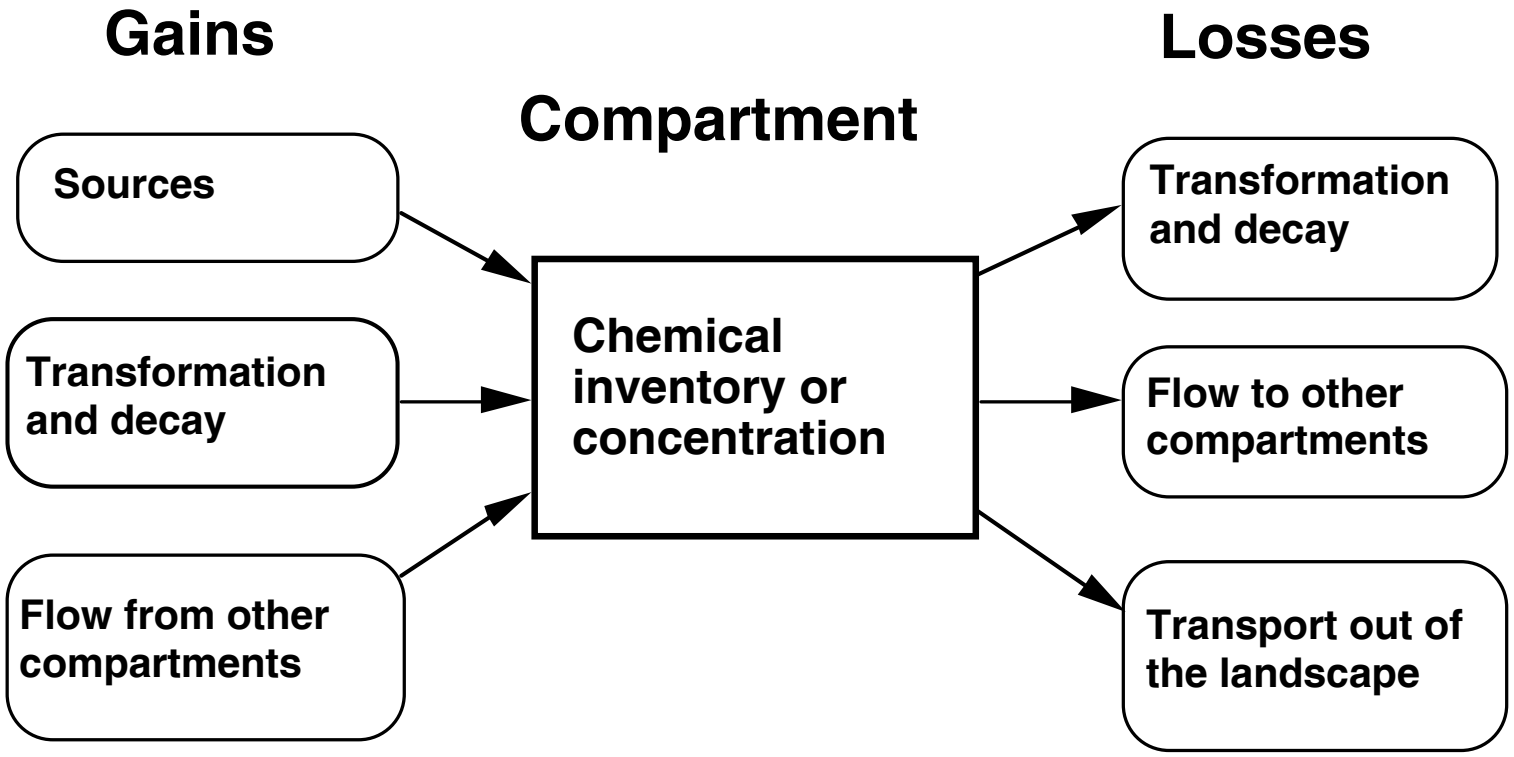

Environmental transport and transformation
(outdoors and indoors)
air
Pesticide use
Exposure
Events
Indoor air
Indoor surfaces
Food
water
soil layers
sediment
Uptake
Biokinetics
Urinary
biomarker

Confronting Exposure Potential

- Persistence
- Proximity
- Mobility



Overall Persistence



$$\text{Inventory (mol)} = \text{Gains} - \text{Losses (mol/d)}$$

$$\text{Pov (d)} = \frac{\text{Inventory (mol)}}{\text{Re action Losses(mol/d)}}$$

Long-Range Transport Potential and Mobility

Characteristic travel distance (CTD)

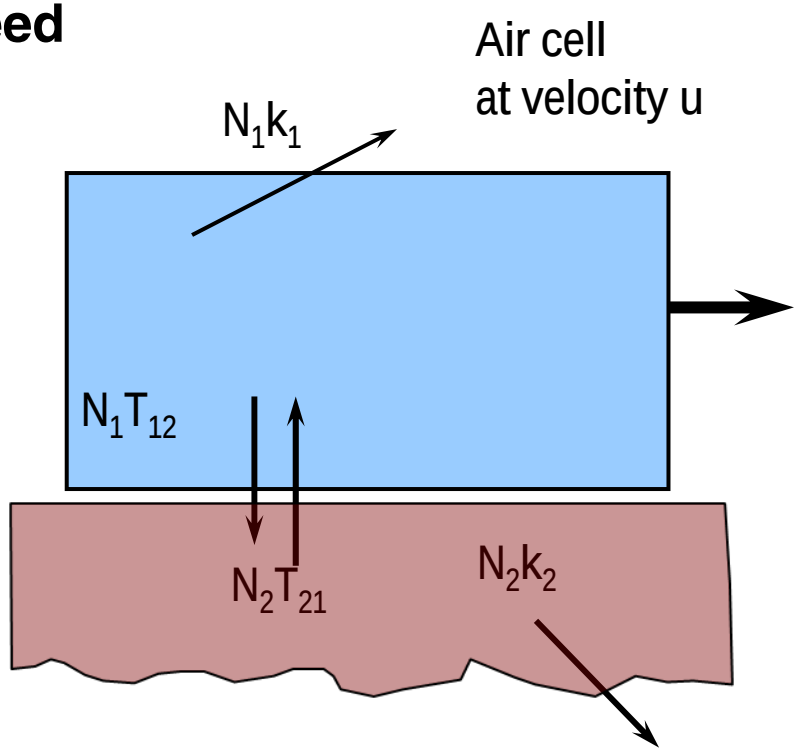
$$CTD = u/k_{effective}$$

u **= long-term average wind speed**

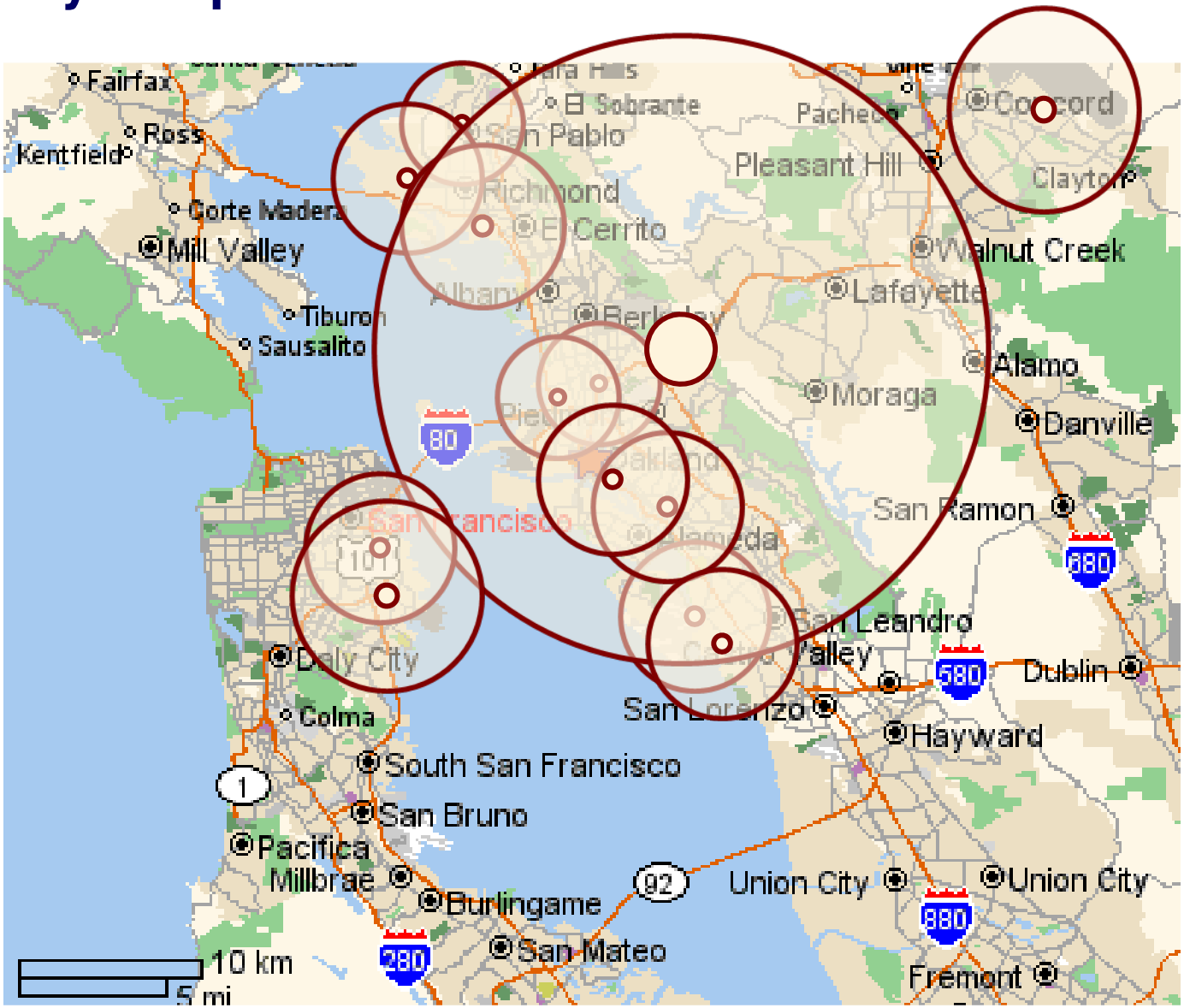
$k_{effective}$ **= effective chemical decay rate**

Mobility = Effective Velocity

Depends on wind velocity & "stickiness



Linking Populations to the "Reach" and Proximity of Specific Pollutant Emissions



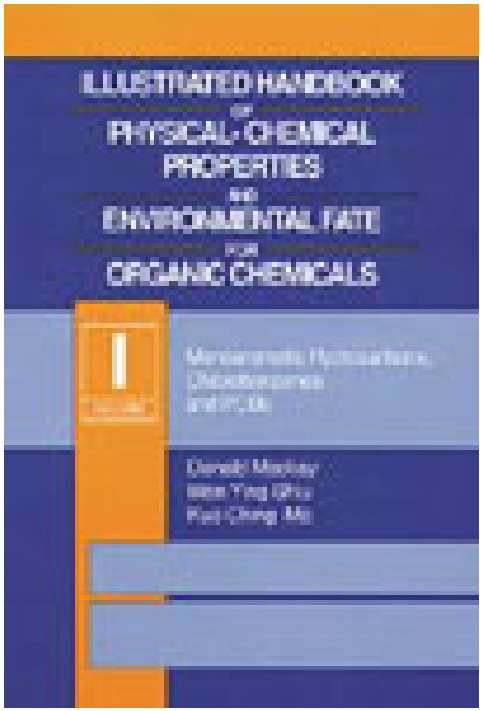
Chemical Properties and Exposure Potential

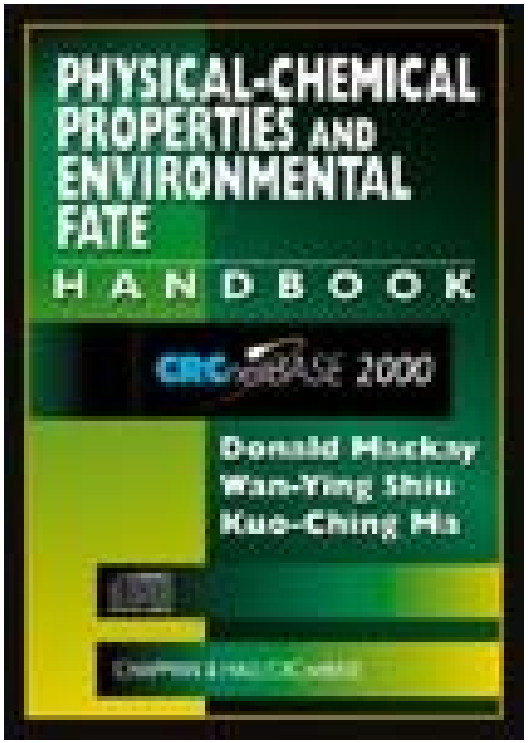
- What chemical properties impact fate and exposure
- The OECD model comparison project
- Intake fraction
- How is exposure linked to POV and LRT?

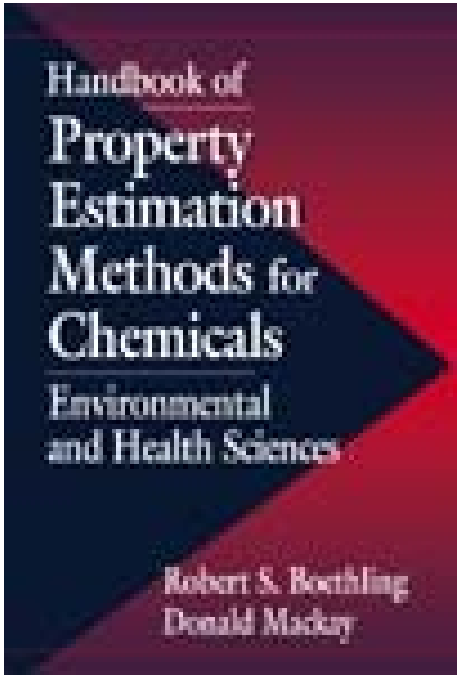
Chemical Properties

- **Provide insight on:**
  - **Fate and transport**
  - **Persistence**
  - **Bioaccumulation potential**
  - **Exposure potential**
- **Important properties**
  - **Air-water partition coefficient**
  - **Octanol-water partition factor**
  - **Transformation rates (air, water, soil)**

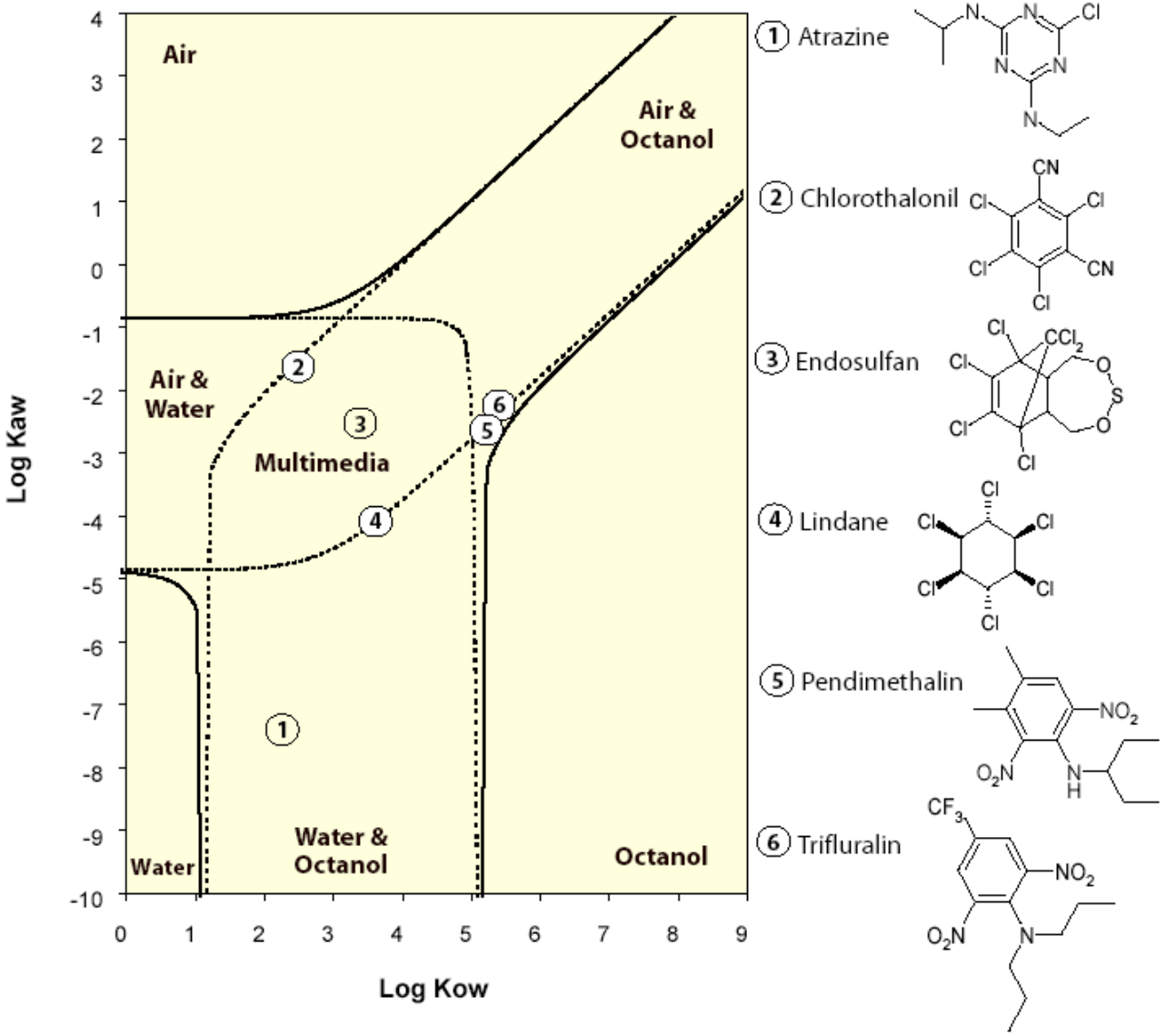
Example References



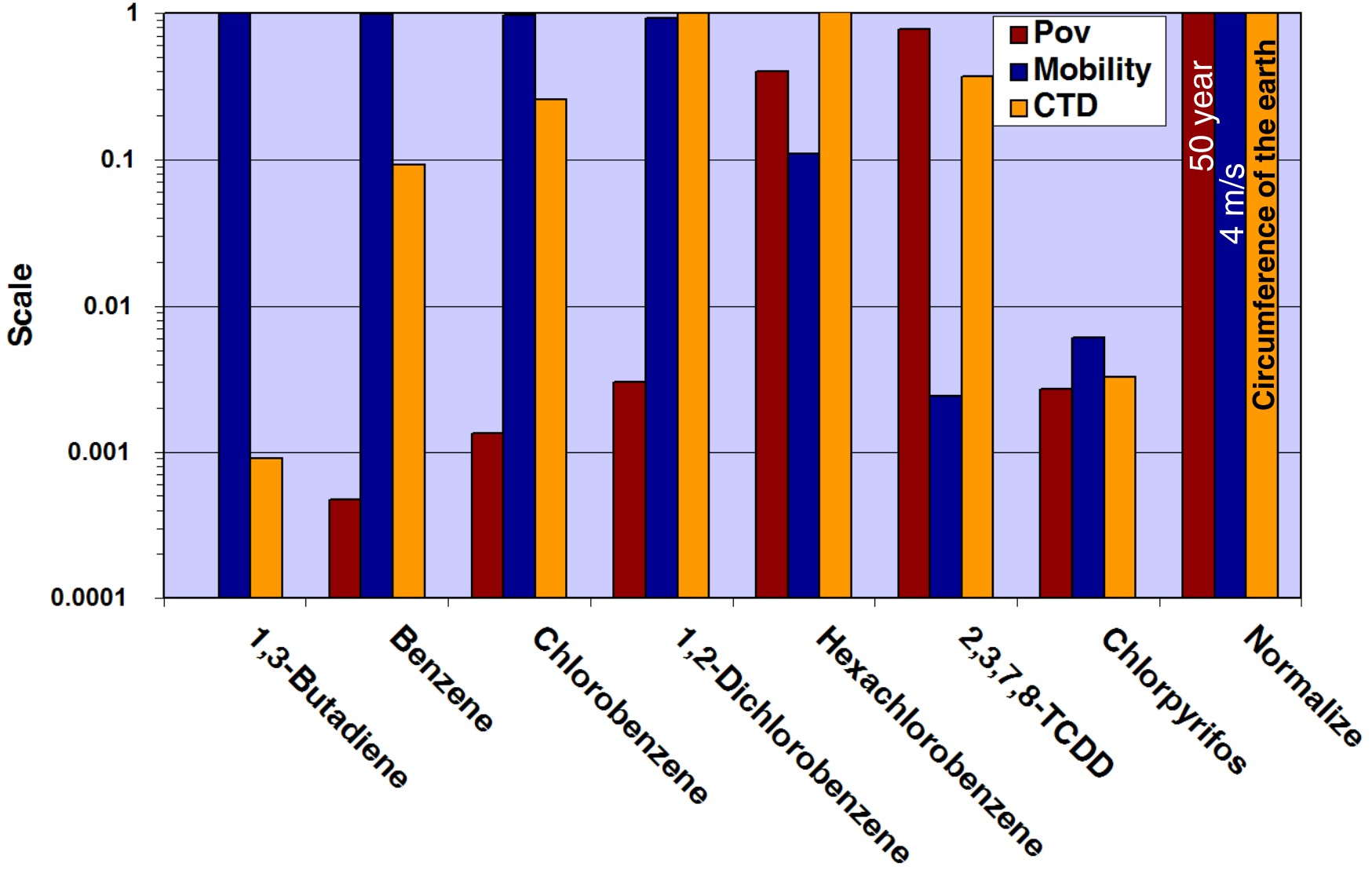




Chemical Properties and Partitioning



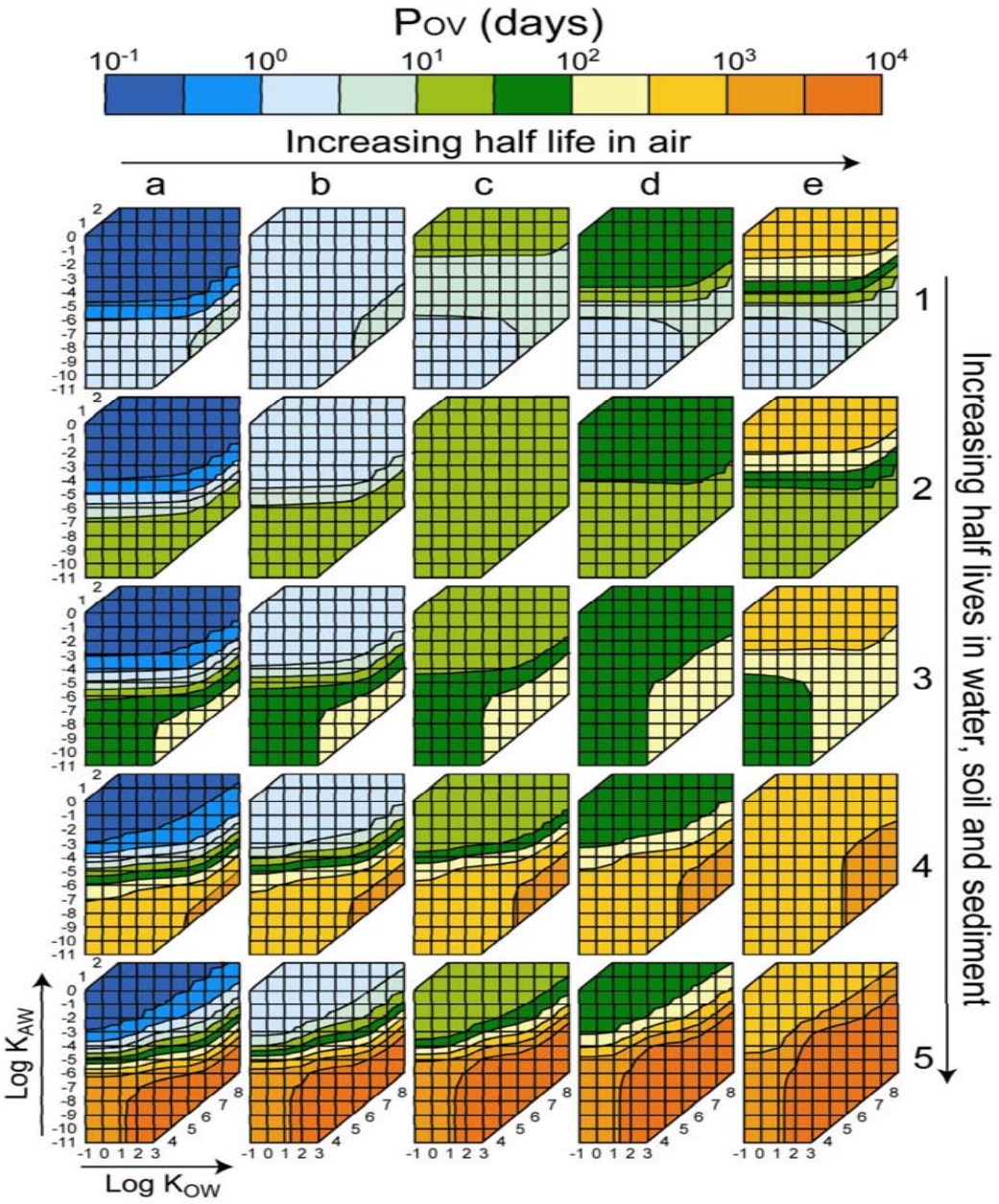
Relative values of Pov, Mobility, and CTD .



OECD Model Comparison

Response surface applied to 9 Models

Here is an example of <u>one</u> outcome mapped against <u>four</u> input parameters over their full range of variation



The Intake Fraction (iF)

$$= \frac{\text{Population Intake}}{\text{Total Emissions}} = \frac{\int_{T_1}^{\infty} \left(\sum_{i=1}^{P} \left(C_i(t) \cdot In_i(t) \right) \right) dt}{\int_{T_1}^{T_2} E(t)\, dt}$$

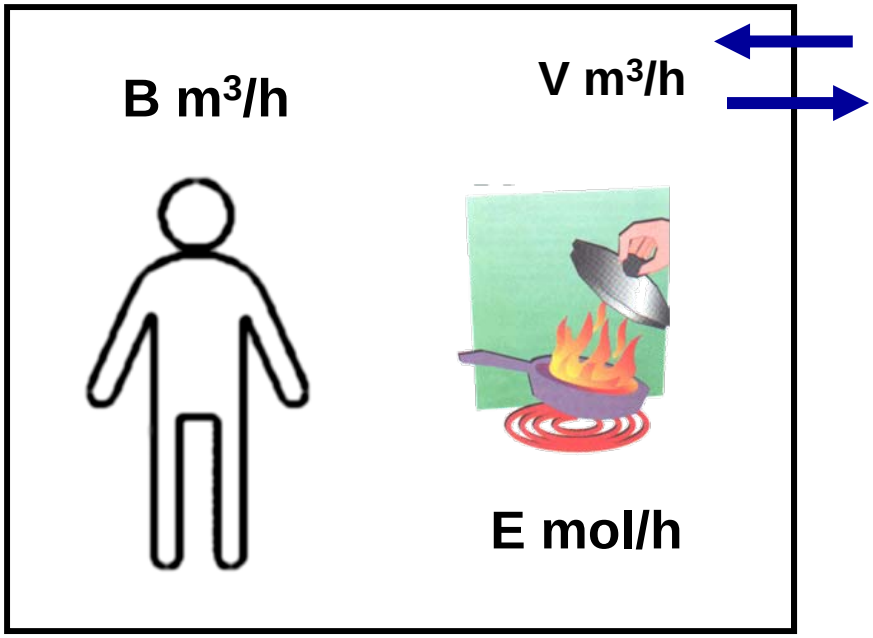
C_i = Concentration (g/m^3)

In_i = Intake rate (m^3/person-day), for example breathing rate

P = Population (persons)

E = Emission rate (g/day)

Intake Fraction Example



Rate of Intake:

$IR = Ca \times B$

Steady State Concentration in Air:

$Ca = E/V$

Loss Rate (Ventilation):

$Loss = Ca \times V$

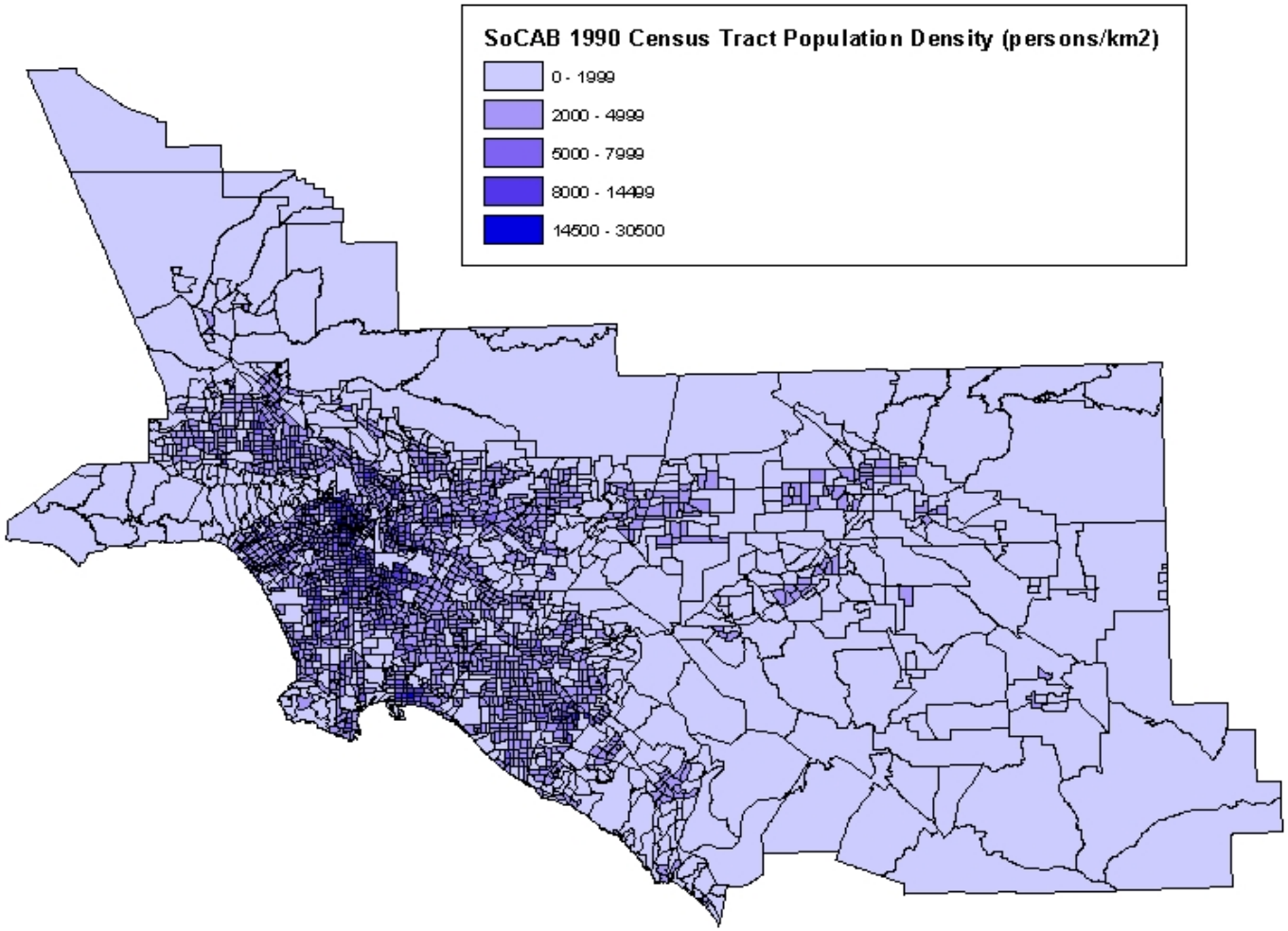
Intake Fraction

$iF = Intake / Emission$

$iF = (Ca \times B) / E$

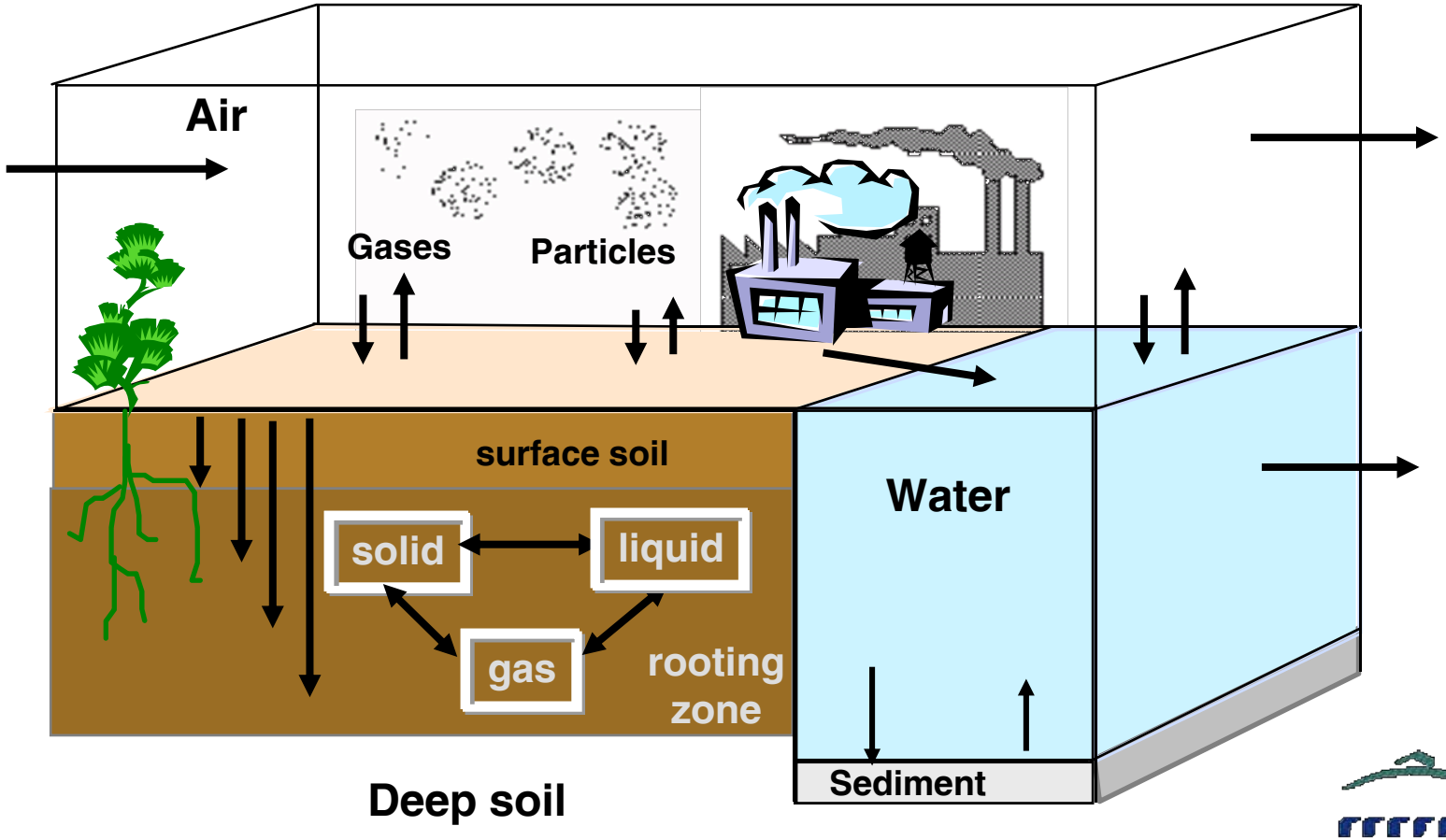
$iF = B/V$

Benzene in the California South Coast Air Basin



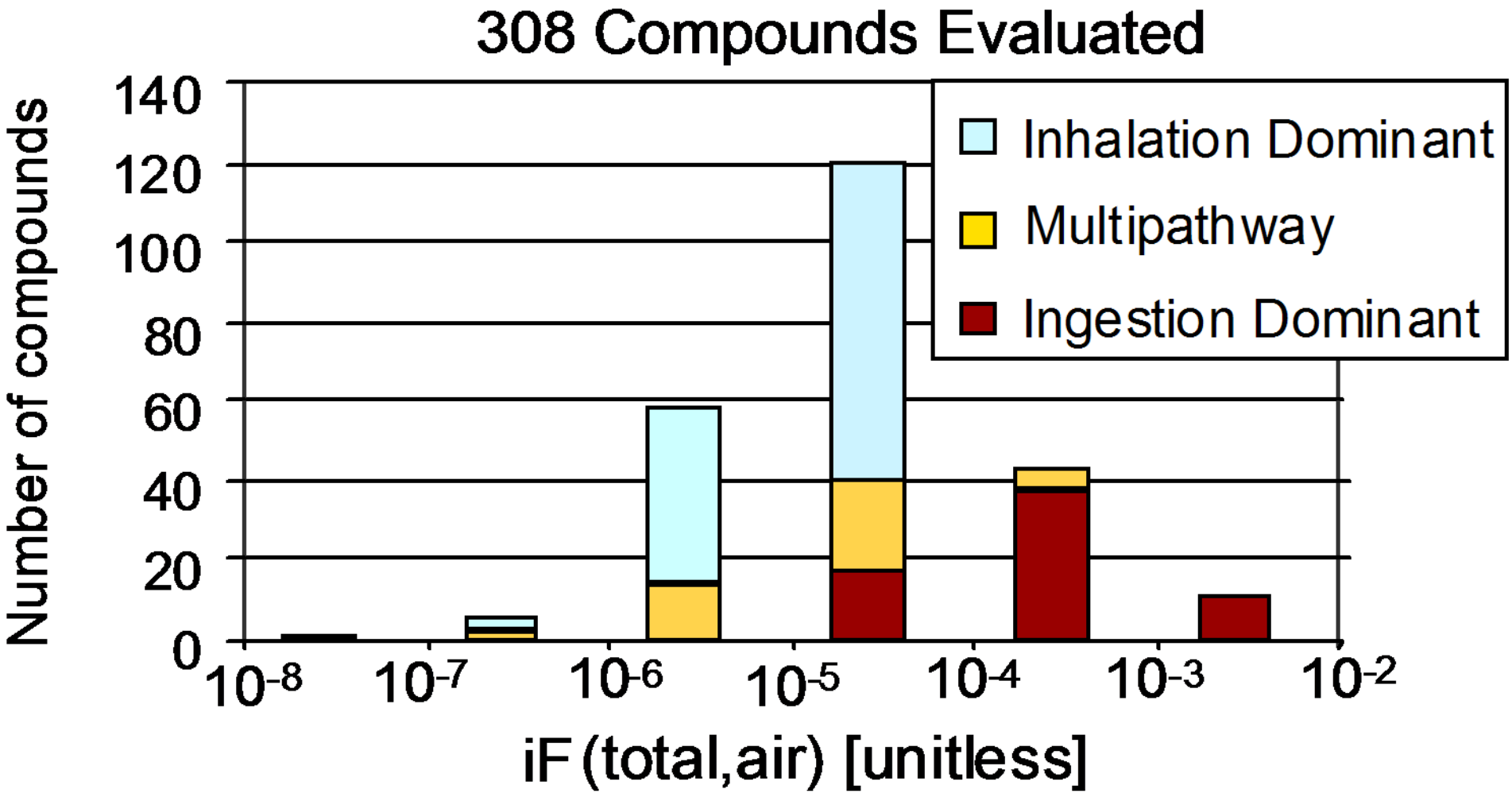
CalTOX

Regional exchange of pollutants among air, soil, water, vegetation etc.

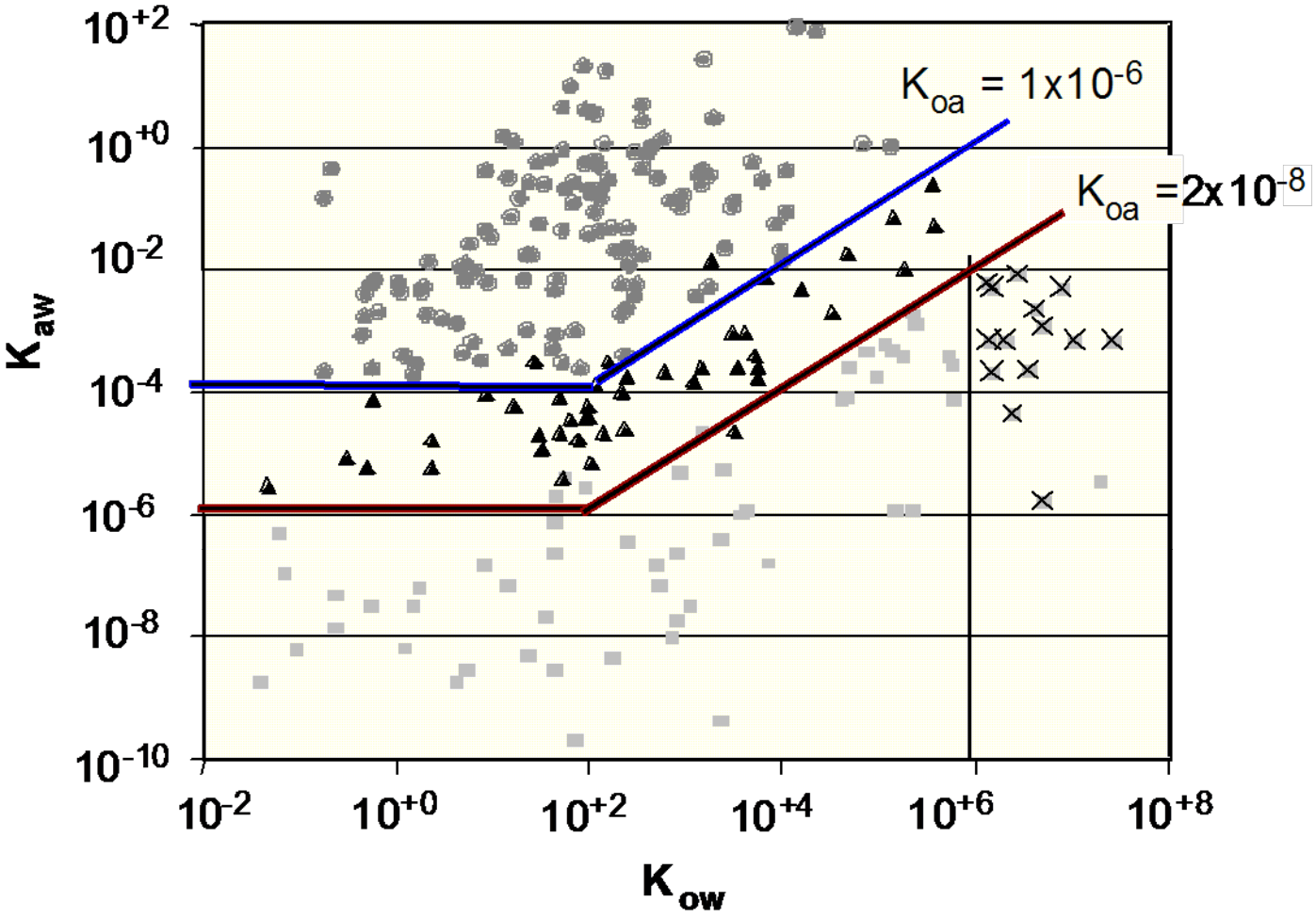


Intake Fraction

(Pathway dependence)



Intake Fraction 308 Chemicals

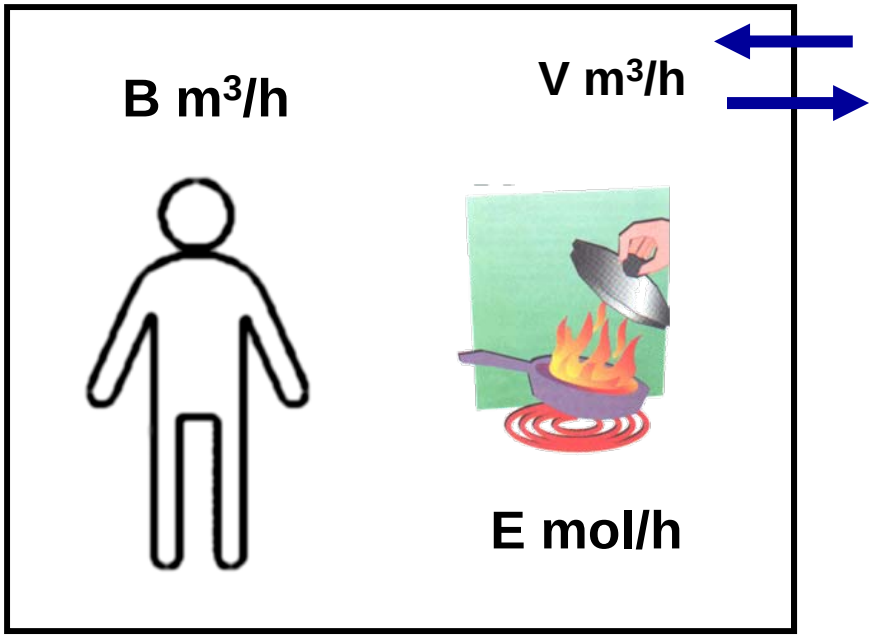


Inhalation Dominant
Multipathway
Ingestion Dominant
Agricultural Products
Meat and Milk

Ranking Tools

- **Exposure depends strongly on:**
  - **Persistence**
    - The longer it lasts the more likely is human intake
    - CTD is dependent on persistence
  - **Proximity (chemical dependent)**
    - CTD defines proximity
  - **Mobility**
    - Mobility of the pollutant
    - Mobility of the population
- **To explore this we use models (CalTOX)**

Characteristic Time of Intake (CTI)



Steady State Concentration in Air:

$Ca = E/V$

Rate of Intake:

$IR = Ca \times B$

Ventilation Rate Loss:

$VR = Ca \times V$

$$iF = (Ca \times B) / (Ca \times V)$$

$$= B / V$$

Intake fraction can be viewed as a competition between the rate of chemical uptake by the population (B) and the rate of clearance from the environment (V)

The relationship between iF and Pov:

$$iF = \frac{Pov}{CTI}$$

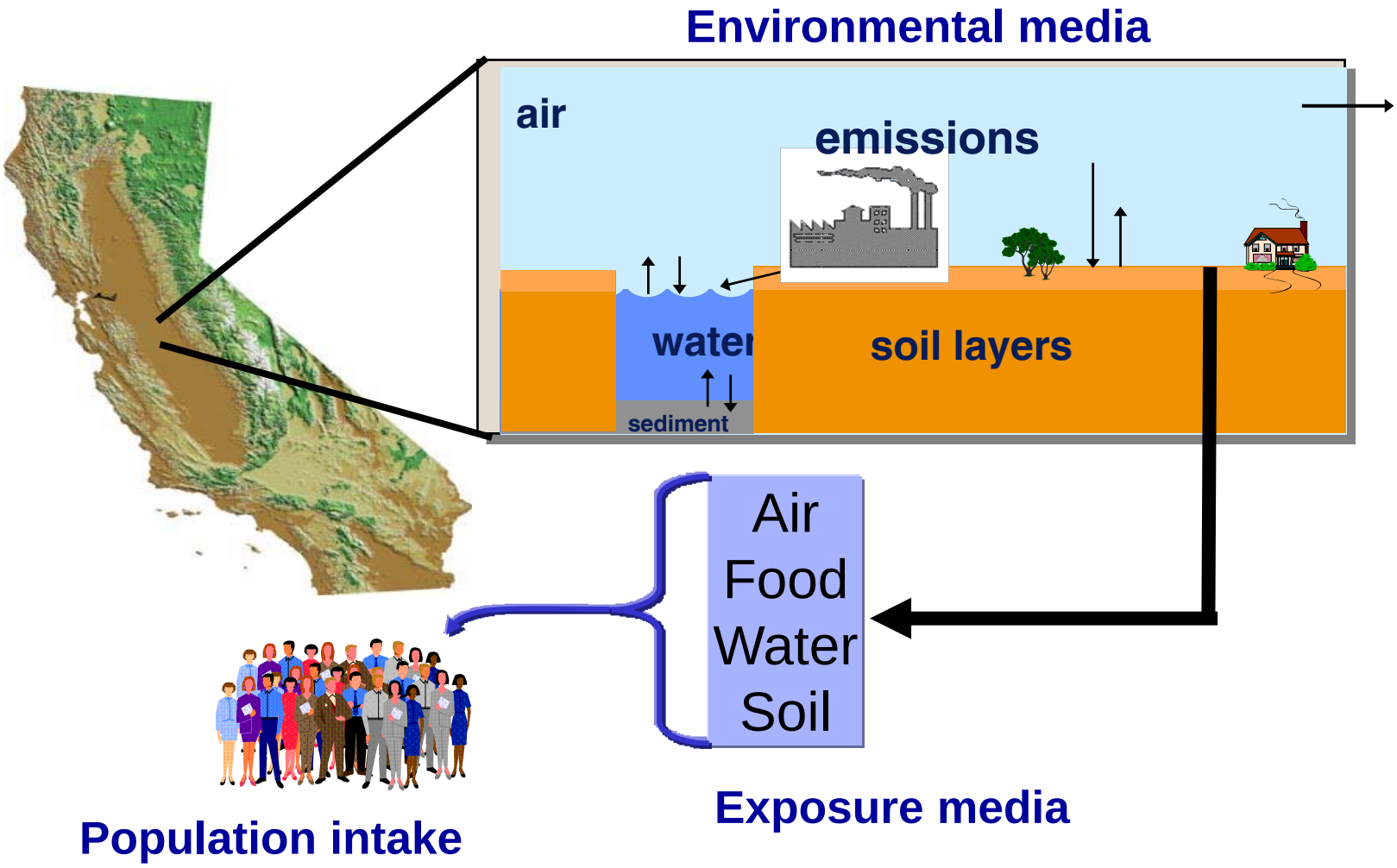
Where, at steady state,

M = Inventory of chemical in the environmental system

Pov = M / emission rate

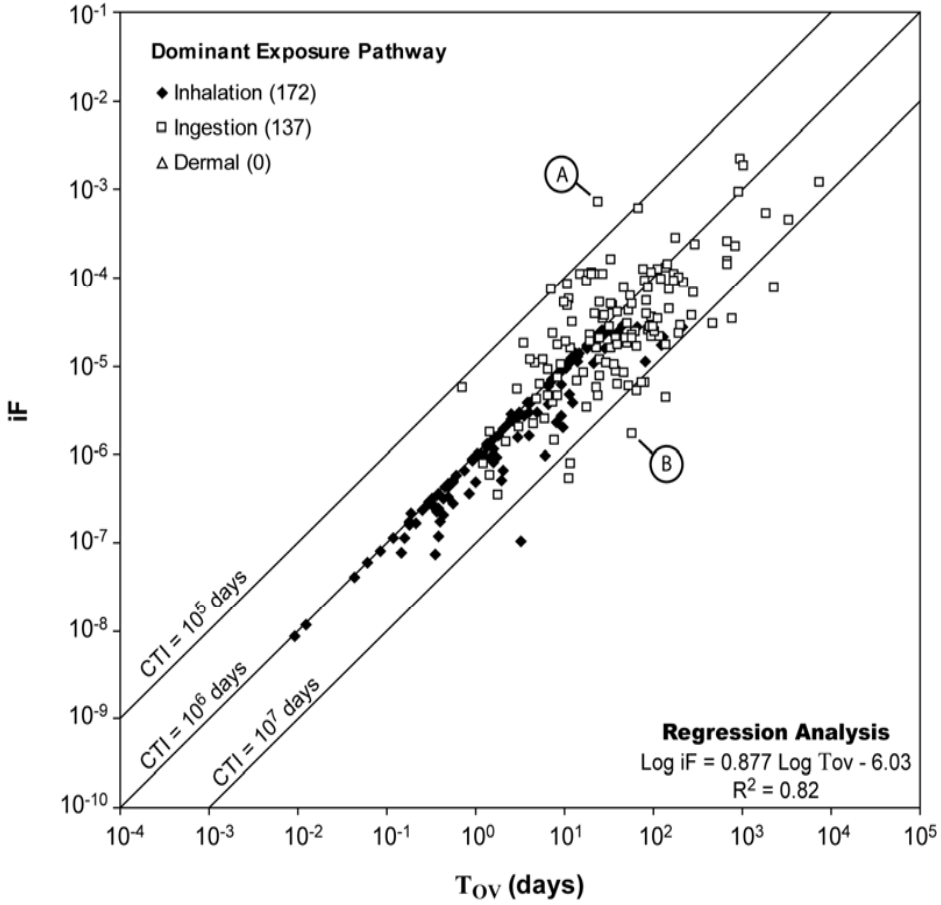
CTI = M / population intake rate

CTI for Regional Multimedia Multipathway Exposures (CalTOX)

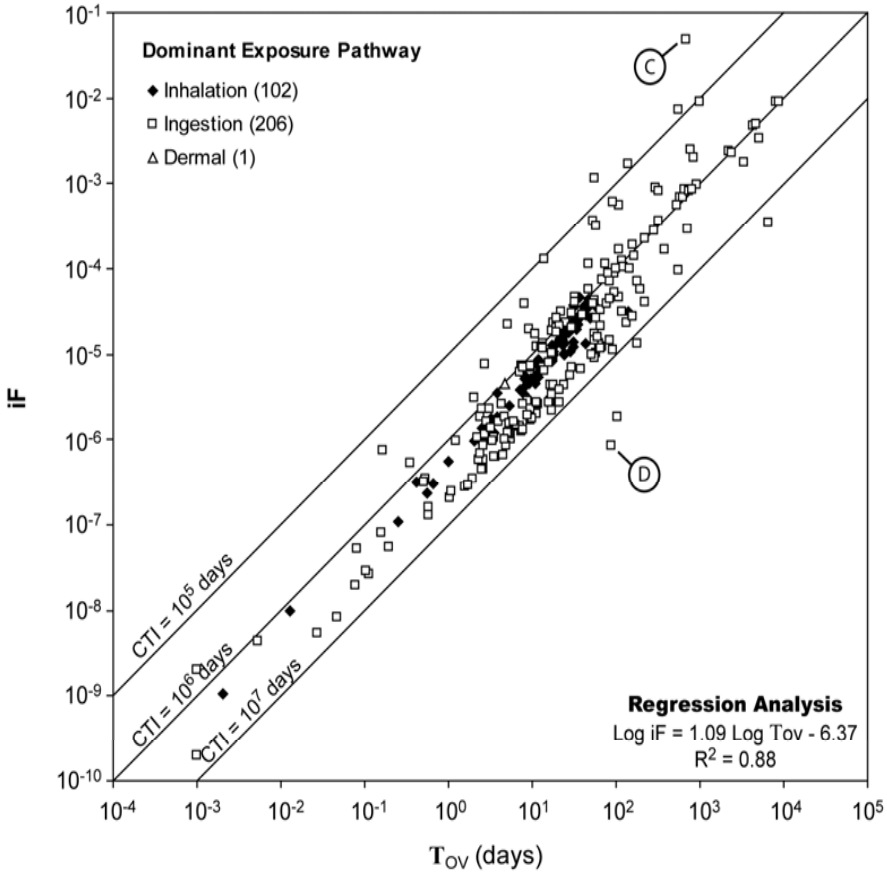


CTI for 315 Chemicals Using CalTOX Applied to North American Region with iF versus Tov (Persistence)

Emissions to Air

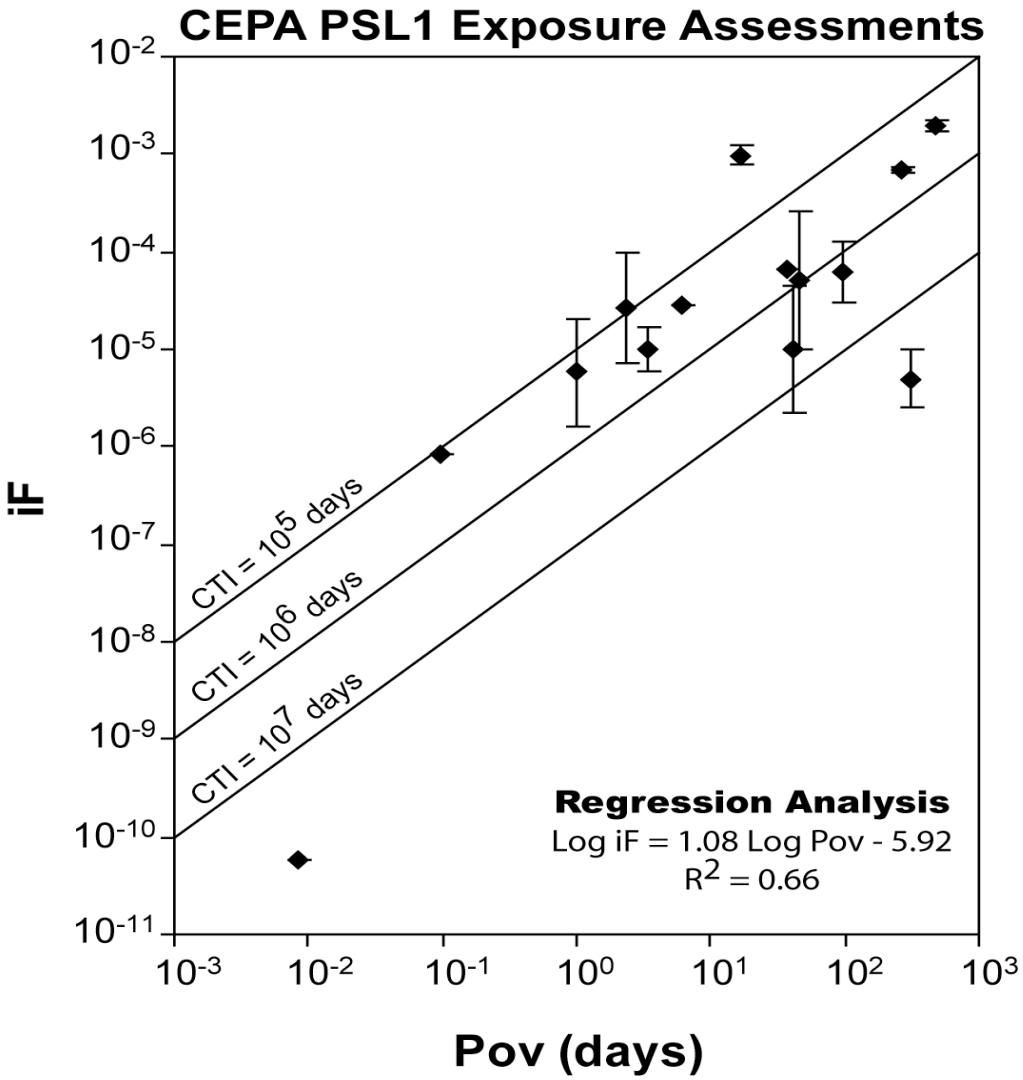


Emissions to Water



iF Based on Canadian Emissions Inventories, Environmental Concentrations and Food Basket Surveys [CEPA PSL1 reports (20010]

Pov (=Tov) estimated from chemical-specific degradation rates in a generic environment



Concluding Points

- Chemical properties tell us much about Pov, mobility, and CTD
- Intake fraction is an effective measure of exposure potential
- Combined modeling/monitoring evaluations indicate that Pov and mobility relate strongly to intake fraction
- For many persistent pollutants, ingestion exposures are dominant and weakly dependent on population proximity